

1-Pentanol
71-41-0 | DTXSID6021741

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 7.31 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.36e-01

Confidence level: 5.83e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Pentanol</div> <div>Measured: 5.01</div> <div>Predicted: 7.31</div>	<div>Image not found</div> <div>Butylamine</div> <div>Measured: 75.9</div> <div>Predicted: 19.9</div>	<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 3.16</div> <div>Predicted: 8.95</div>
<div>Image not found</div> <div>1-Hexanol</div> <div>Measured: 10.2</div> <div>Predicted: 11.9</div>	<div>Image not found</div> <div>4-Vinylpyridine</div> <div>Measured: 15.1</div> <div>Predicted: 43.8</div>	